NASA TECHNICAL MEMORANDUM

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COLUMN DENSITIES RESULTING FROM SHUTTLE SUBLIMATOR/EVAPORATOR OPERATION

Robert J. Naumann
(NASA-TH-X-64794) COLUMN DENSITIES
RESULTING FROM SHUTTLE
SUBLINATOR/EVAPORATOR OPERATION (NASA)
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	vapor form through a superson the point of view of the possible located at the tail and directed density will be less than 10 ¹² m longitudinal axis. The molecules ex This contribution from molecules ex molecules were expelled. Sum	e interference to astronomical along the Shuttle longitudinal a colecules/cm ² at viewing angles les in the trail will diffuse rapic pelled on the previous orbit is the inverse square root of the ming the contributions from eacolumn density of 5×10^9 molecum return flux from water molecular	day has been investigated from experiments. If the nozzle is exis, the resulting column starger than 48 deg above the edly. The column density 1.3 × 10 ⁸ molecules/cm ² . In a number of orbits since the each orbit over a 30-day cules/cm ² along a perpendicular

The molecular backscatter from atmospheric molecules is also calculated. If the plume is directed into the flight path, the column density along a perpendicular is found to be 1.5×10^{11} molecules/cm². The return flux is estimated to be of the order of 10^{12} molecules/ $\mathrm{cm}^2/\mathrm{sec}$ at the stagnation point. With reasonable care in design of experiments to protect them from the backscatter flux of water molecules, the expulsion of 100 lb/day does not appear to create an insurmountable difficulty for the Shuttle experiments.

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TECHNICAL MEMORANDUM X-64794

COLUMN DENSITIES RESULTING FROM SHUTTLE SUBLIMATOR/EVAPORATOR OPERATION

INTRODUCTION

A proposal has been made to dispose of the 100 lb of water $(H_2O)/day$ generated from Shuttle fuel cell operation by a more or less continuous overboard dump through a supersonic nozzle after the H_2O has been converted into gaseous form via the sublimator/evaporator. Astronomers desire a column density of no more than 10^{12} molecules/cm² so that the induced atmosphere will be optically thin at all wavelengths. The purpose of this study is to determine the column density resulting from the H_2O vent.

The plume origin is taken to be at (x_0, y_0) , with the plume axis along the x-axis $(x_0 = 13.7 \text{ m}, y_0 = 4.6 \text{ m})$, as shown in Figure 1. The line of sight \overrightarrow{S} originates at the origin and makes angle γ with the x-axis. To simplify the geometry, only the worst case situation in which the line of sight \overrightarrow{S} is in the x-y plane will be considered.

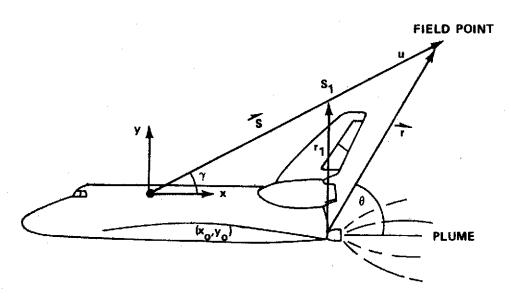


Figure 1. Plume geometry.

The plume distribution has been determined semi-empirically to have the form

$$\phi(\mathbf{r}, \theta) = \frac{N_c(\cos \theta)^n}{r^2}, \quad (\theta < \pi/2)$$

where n = 6.272. $\phi(r, \theta)$ is the molecular current along a radius r making angle θ with the plume axis. The normalization constant N is determined by requiring

$$\dot{N}_{T} = \int_{\text{hemisphere}} \phi(\mathbf{r}, \theta) dA$$

where $\dot{N}_{_{\mathbf{T}}}$ is the total molecular flow rate.

Since $dA_{\parallel} = 2\pi r^2 \sin \theta d\theta$, the integral becomes

$$\dot{N}_{T} = \frac{2\pi N_{c}}{n+1} ,$$

from which

$$N_{c} = \frac{(n+1)}{2\pi} \dot{N}_{T} .$$

ANALYSIS

The number density at any (r, θ) is given by dividing the current $\phi(r, \theta)$ by the mean radial velocity of the molecules. This velocity is given by

$$v = \sqrt{\frac{2\gamma RT}{(\gamma-1)M}} = 1003 \text{ m/sec}$$

for H_2O at $T = 273^{\circ}$ K.

Therefore,

$$N(r, \theta) = \frac{(n+1) \dot{N}_{T}(\cos \theta)^{n}}{2\pi v r^{2}}, \qquad (\theta < \pi/2)$$

The column density is found by integrating $N(r, \theta)$ along the line of sight (LOS),

$$n_{c} = \int_{s_{t}}^{\infty} N(r, \theta) ds$$

where s_i is the point at which the LOS \overline{S} intersects the nozzle plane. Let $u = s - s_i$. From the law of cosines,

$$\mathbf{r}^2 = \mathbf{r}_i^2 + \mathbf{u}^2 + 2\mathbf{r}_i\mathbf{u}\sin\gamma \quad .$$

From the law of sines,

$$\cos \theta = \frac{\mathbf{u}}{\mathbf{r}} \cos \gamma$$
.

Finally,

$$n_{c} = \frac{(n+1) \dot{N}_{T}}{2\pi v} \int_{0}^{\infty} \frac{(u \cos \gamma)^{n}}{r^{n+2}} du$$

Let
$$x = u/r_1$$
;

$$n_c = \frac{(n+1) \dot{N}_T}{2\pi v r_1} \int_0^{\infty} \frac{(x \cos \gamma)^n dx}{(x^2 + 2x \sin \gamma + 1)^{\frac{n+2}{2}}}$$

where

$$r_1 = x_0 \tan \gamma - y_0$$

The integration is easily carried out by the Gauss-Leguerre method using eight points. The results are shown in Table 1. From the plot of $n_{\rm c}$ as a function of angle in Figure 2, it can be seen that the 10^{12} molecules/cm² is violated for look angles smaller than 48 deg from the tail.

TABLE 1. COLUMN DENSITIES

γ (deg)	(cm)	Ι (δ)	$ \begin{array}{c} $	log n
0	460	0.443	1.95 (14)	14.29
10	701	0.284	8.22 (13)	13.91
20	958	0.160	3.39 (13)	13.53
30	1 250	0.764	1.24 (13)	13.09
40	1 609	0.0294	3.70 (12)	12.57
50	2 092	0.00850	8.24 (11)	11.91
60	2 832	0.00158	1. 13 (11)	11.05
70	4 224	0.000135	6.48 (9)	9.81
80	8 229	1.84 (-6)	4.54 (7)	7.65
. 85	16 119	2.41 (-8)	3.03 (5)	5.48

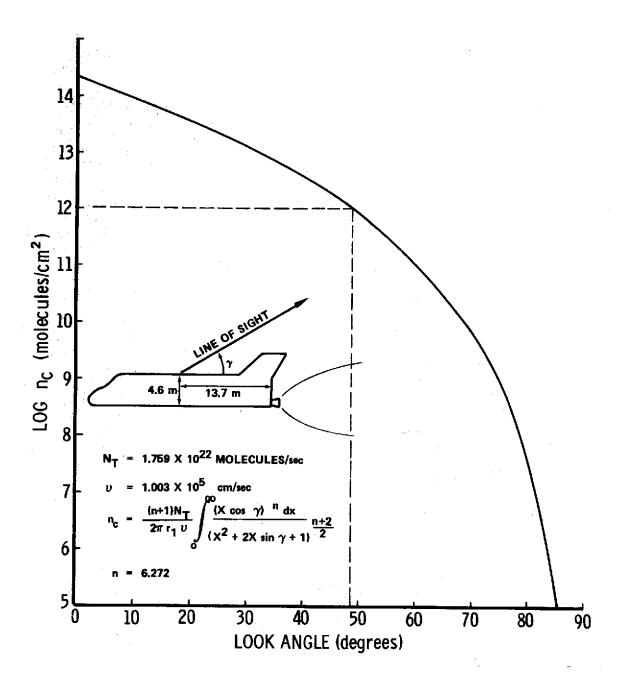


Figure 2. Column density versus look angle.

ORBITAL ACCUMULATION

Water molecules expelled from the Shuttle will have approximately $8\,$ km/sec relative velocity to the atmospheric molecules. The collision rate will be

$$\dot{Q} = N_a \sigma_a v_a$$

where

$$N_c = 1.5 \times 10^{14} \text{ molecules/m}^3 \text{ at } 420 \text{ km}$$

$$\sigma_{a} = 1.04 \times 10^{-19} \text{ m}^{2}$$

$$v_{s} = 8 \times 10^3 \text{ m/sec}$$

$$\dot{Q} = 0.125/\text{sec}$$

or the time between collisions is 8 sec.

The mean distance from the spacecraft before collision occurs is $v/\dot{Q}\approx 8$ km. Since the water molecules have comparable mass to the atmospheric molecules, the velocity change from collision will be very large. After a few collisions, the expelled molecules will be completely randomized and their dispersion will be controlled by a diffusion process. The accumulation of H_2O along the orbital path will be investigated.

Consider the H_2O trail left by the Shuttle to be initially a line of molecules along the orbital path with a linear density λ molecules/cm. Next, consider a cross section perpendicular to this line with thickness $d\ell$. The number of molecules in this volume is $\lambda d\ell$. Let $\sigma(r$, t) be the area density in this cross section (molecules/cm²). The volume density N(r, t) is related to $\sigma(r$, t) by

$$\sigma(\mathbf{r}, t) = N(\mathbf{r}, t) d\ell$$

Assuming azimuthal symmetry, the molecules will spread in time according to the diffusion equation

$$\frac{\partial \sigma}{\partial t} \stackrel{(\mathbf{r}, t)}{=} \nabla \cdot \alpha \nabla \sigma(\mathbf{r}, t)$$
.

If α is not a function of r, this equation reduces to

$$\frac{\partial \sigma}{\partial t}$$
 (r, t) = $\frac{\alpha}{r} \frac{\partial}{\partial r}$ (r $\frac{\partial \sigma}{\partial r}$ (r, t))

where α is the diffusion coefficient given by

$$\alpha = \frac{\lambda_{\mathbf{f}}^{\mathbf{KT}}}{\mathbf{m}\nabla} = \frac{1}{\sqrt{2 N_{\mathbf{a}} \sigma_{\mathbf{a}}}} \sqrt{\frac{\pi \mathbf{KT}}{8\mathbf{m}}}$$

where λ_f is the mean free path after randomization, K is Boltzmann's constant, m is the molecular mass, and T is the temperature.

The solution to the diffusion equation in polar coordinates has the form

$$\sigma(\mathbf{r}, \mathbf{t}) = \frac{C}{2\alpha t} e^{-\mathbf{r}^2/4\alpha t}$$

where C is a normalization constant. This constant is determined by requiring

$$\int_{0}^{\infty} \sigma(\mathbf{r}, t) 2\pi r d\mathbf{r} = \lambda d\ell$$

where $\lambda d\boldsymbol{\ell}$ is the total number of molecules in the section under consideration. Carrying out the integration results in

$$2\pi C = \lambda d\ell$$

Therefore,

$$\sigma (\mathbf{r}, \mathbf{t}) = \frac{\lambda d\ell}{4\pi\alpha t} e^{-\mathbf{r}^2/4\alpha t}$$

and

$$N(r, t) = \frac{\lambda}{4\pi\alpha t} e^{-r^2/4\alpha t}$$
.

The column density, looking perpendicular to the flight path, is given by

$$n_c = \int_0^\infty N(r, t) dr = \frac{\lambda}{4\pi\alpha t} \int_0^\infty e^{-r^2/4\alpha t} dr$$

$$n_{c} = \frac{\lambda}{4\pi^{\frac{1}{2}}\alpha^{\frac{1}{2}}t^{\frac{1}{2}}}$$
.

The linear density λ is just the expulsion rate of molecules $\dot{N}_{\rm T}$ divided by the velocity of the spacecraft relative to the atmosphere, or

$$\lambda = \frac{1.76 \times 10^{22}}{8 \times 10^5} = 2.2 \times 10^{16} \text{ molecules/cm}$$

Assuming the nozzle is directed such that the molecules are placed behind the spacecraft, they will not be reencountered until one orbit later, or $t\approx 6\,000$ sec.

The diffusion coefficient is

$$\alpha = \frac{\left(\frac{\pi}{8} \frac{8.32 \times 10^7 \text{ ergs/mol/deg } 270}{8 \text{ mol/cm}^3 \text{ mol/cm}^3}\right)^{\frac{1}{2}}}{\sqrt{2} \left(1.5 \times 10^8 \text{ mol/cm}^3\right) \left(1.04 \times 10^{-15} \text{ cm}^2\right)}$$

$$= 1.00 \times 10^{11} \text{ cm}^2/\text{sec} .$$

After one period, the column density is

$$n_{c_1} = \frac{2.2 \times 10^{16}}{4\sqrt{\pi} (1.00 \times 10^{11} 6000)^{\frac{1}{2}}} = 1.26 \times 18^8 \text{ mol/cm}^2$$

This is the contribution from the first orbit. One orbit later, this will have been reduced to

$$\mathbf{n_{c_2}} = \frac{\mathbf{n_{c_1}}}{2^{\frac{1}{2}}}$$

and the total column density is

$$n_c = n_c \sum_{n=1}^{N} \left(\frac{1}{n^{\frac{1}{2}}}\right)$$

This series does not converge as $N\to\infty$; however, it increases slowly. Other factors ultimately place an upper bound on the increase in column density. First, the diffusion coefficient increases with altitude. Second, oblateness perturbations and earth rotation prevent the spacecraft from traversing the same path through the atmosphere on subsequent orbits. For a 7-day mission, the number of orbits is ~100 and the series sum is ~18.

For 30 days, N \approx 432 and the series sum is ~40. This is probably a worst case estimate because of the preceding considerations, but the maximum effect from orbital accumulation for a 30-day mission is 5×10^9 molecules/cm².

The molecular impingement resulting from flying through the molecules expelled from the previous pass is given by N(0 , 6 000 sec) v $_{\rm a}$ or

$$Q_{\text{ret}} = \frac{\lambda v_{\text{a}}}{4\pi\alpha t} = \frac{2.2 \times 10^{16} \text{ 8} \times 10^{5}}{4\pi (1.0 \times 10^{11}) (6 000)}$$
$$= 3.67 \times 10^{8} \text{ mole/cm}^{2} \text{ sec} .$$

Previous orbits will each contribute 1/n times this amount. Summing 1/n over 432 orbits yields

$$Q_{ret} = 2.2 \times 10^9 \text{ molecules/cm}^2 \text{ sec}$$

at the stagnation point.

MOLECULAR BACKSCATTER

If the nozzle is oriented so that the expelled molecules are directed in front of the spacecraft, the spacecraft will fly through its own cloud as these molecules collide with atmospheric molecules. The major contribution will come from those molecules that collide fairly close to the spacecraft before they become randomized. Therefore, a single collision model is more appropriate than the diffusion model developed previously.

For simplicity, let the expelled molecules leave the spacecraft with velocity v_r in a parallel beam along the x-axis. Their mean free path relative to the spacecraft is $x_{\lambda} = v_{\alpha} (N_{\alpha} \sigma_{\alpha} v_{\alpha})^{-1}$. The probability of a molecule colliding with an atmospheric molecule in the interval dx at distance x is

$$P(x) dx = Po(x) [1 - Po (dx)]$$

where Po(x) is the survival probability after traversing distance x. This is given by Poisson statistics as

$$Po = e^{-x/x}\lambda$$

Therefore,

$$P(x) dx = \frac{\frac{N_a \sigma_a v_a}{v_r} exp \left(-N_a \sigma_a v_a x/v_r\right) dx}{v_r} dx$$

The probability that a molecule will be scattered into solid angle $\,d\!\omega$ is given by

$$\frac{1}{\sigma_a} \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \right)_{\theta} \mathrm{d}\omega$$
 .

The differential scattering cross section in the center of mass system is isotropic and is given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathbf{c/m}} = \frac{\sigma_{\mathbf{a}}}{4\pi}$$
.

Since the velocity of the molecules relative to the spacecraft is small compared to the velocity relative to the atmospheric molecules, the expelled molecules will be considered at rest in the lab system. Also, the expelled molecules will be considered to have the same mass as the atmospheric molecules. The differential cross section transforms according to

$$\left(\frac{d\sigma}{d\Omega}\right)_{lab} 2\pi \sin\theta \ d\theta = \left(\frac{d\sigma}{d\Omega}\right)_{c/m} 2\pi \sin\theta * d\theta *$$

where θ^* is the scattering angle in the c/m system and θ is the angle at which the stationary molecule is scattered relative to the colliding molecule. This angle transforms according to

$$\theta^* = \pi - 2\theta$$

Therefore,

$$\frac{1}{\sigma_{a}} \left(\frac{d\sigma}{d\Omega} \right)_{\theta} = \frac{4 \cos \theta}{\sigma_{a}} \left(\frac{d\sigma}{d\Omega} \right)_{c/m} = \frac{\cos \theta}{\pi} .$$

The scattered velocity is seen from the Figure 3 diagram.

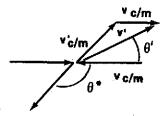


Figure 3. Collision geometry for molecules emanating from the spacecraft colliding with atmospheric molecules.

If the two particles have equal mass, $v_{c/m} = v_a/2$. The velocity in the lab system is found by adding $v_{c/m}$ to the x component.

$$v' = \begin{pmatrix} \frac{v_a}{2} - \frac{v_a}{2} \cos \theta^* \\ -\frac{v_a}{2} \sin \theta^* \end{pmatrix}$$

from which

$$v'^2 = \frac{v^2}{2} (1 - \cos \theta^*)$$

Using $\theta^* = \pi - 2\theta$

$$v^{12} = \frac{v^2}{2} (1 + \cos 2\theta) = v_a^2 \cos^2 \theta$$

or

$$v^{\dagger} = v_a \cos \theta$$

The number of molecules per unit time scattered from dx into solid angle d ω is given by

$$\dot{N}_{T} P(x) dx \frac{1}{\sigma_{a}} \left(\frac{d\sigma}{d\Omega}\right)_{\theta} d\omega$$
 (see Figure 4)

The molecular flux is this number divided by the area subtended by $\,\mathrm{d}\omega$, which is $(r^2+x^2)\,\,\mathrm{d}\omega$. The contribution to the number density is this flux divided by the velocity perpendicular to the area subtended by $\,\mathrm{d}\omega$. Therefore,

$$dN'(\mathbf{r}) = \frac{\dot{N}_T P(x) dx}{(\mathbf{r}^2 + \mathbf{x}^2) \mathbf{v}' \sigma_a} \left(\frac{d\sigma}{d\Omega}\right)_{\theta}$$

Inserting the expressions for $\left(\frac{d\sigma}{d\Omega}\right)_{\theta}$, P(x)~dx , and ~v' , gives

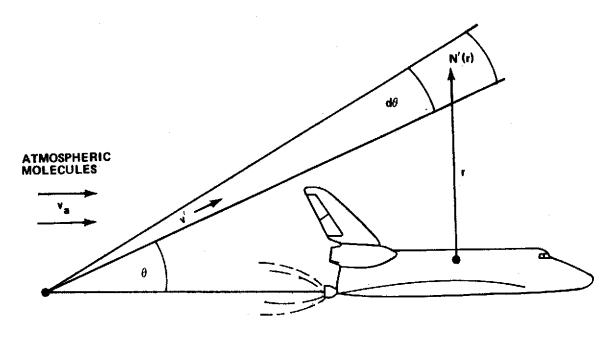


Figure 4. Contribution to column density from molecules backscattered by atmospheric collisions.

$$dN'(r) = \frac{N_a \sigma_a v_a dx \dot{N}_T \cos \theta \exp \left(-N_a \sigma_a v_a x/v_r\right)}{\pi v_r (r^2 + x^2) v_a \cos \theta}$$

The column density contribution from dx is given by

$$dn_c = \int_{\mathbf{r}_0}^{\infty} dN'(\mathbf{r}) d\mathbf{r}$$

$$dn_{\mathbf{c}} = \frac{\dot{\mathbf{N}}_{\mathbf{T}} \mathbf{N}_{\mathbf{a}} \sigma_{\mathbf{a}} dx \exp \left(-\mathbf{N}_{\mathbf{a}} \sigma_{\mathbf{a}} \mathbf{v}_{\mathbf{a}} \mathbf{x} / \mathbf{v}_{\mathbf{r}}\right)}{\pi \mathbf{v}_{\mathbf{r}}} \int_{\mathbf{r}_{\mathbf{0}}}^{\infty} \frac{d\mathbf{r}}{\mathbf{r}^{2} + \mathbf{x}^{2}}$$

In the lim $r_0 \rightarrow 0$, this becomes

$$d n_{c} = \frac{N_{a} \sigma_{a} \dot{N}_{T} \exp(-N_{a} \sigma_{a} v_{a} x/v_{r}) dx}{2 v_{r} x}$$

The column density is found by

$$n_{c} = \int_{x_{o}}^{\infty} dn_{c}$$

Let $u = x/x_0$. x_0 becomes

$$n_{c} = \frac{N_{a} \sigma_{a}}{2 v_{r}} \int_{1}^{\infty} \frac{e^{-\beta u}}{u} du$$

where

$$\beta = N_a \sigma_a v_a x_o u/v_r$$
.

Integrating yields

$$n_{\mathbf{c}} = \frac{\overset{\mathbf{N}_{\mathbf{a}} \overset{\mathbf{\sigma}_{\mathbf{a}} \overset{\mathbf{N}}{\mathbf{T}}}}{2 v_{\mathbf{r}}} \quad \left(-\gamma - \ln \beta + \beta - \frac{\beta^2}{2 \cdot 2!} + \frac{\beta^3}{3 + 3!} + \ldots \right)$$

where $\gamma = 0.577$ (Euler's constant).

$$\beta = 1.5 \times 10^{14} \frac{\text{molecule}}{\text{m}^3} \quad 1.04 \times 10^{-19} \frac{\text{m}^2}{\text{molecule}} \frac{8 \text{ km/sec}}{1 \text{ km/sec}} \quad 13.7 \text{ m}$$

$$\beta = 9.1 \times 10^{-6}$$

Therefore,

$$n_{c} = \frac{\left(1.5 \times 10^{8} \frac{\text{mol}}{\text{cm}^{3}}\right) \left(1.04 \times 10^{-15} \frac{\text{cm}^{2}}{\text{mol}}\right) \left(1.76 \times 10^{22} \frac{\text{mol}}{\text{sec}}\right) (11.03)}{2(1.00 \times 10^{5} \text{ cm/sec})}$$

$$n_c = 1.5 \times 10^{11} \text{ mol/cm}^2$$

= $1.3 \times 10^{12} \text{ mol/cm}^2/\text{sec}$

The impingement on the spacecraft from the backscatter is given approximately by

$$Q_{\text{back}} = \frac{\frac{N_{\text{a}} \sigma_{\text{a}} \dot{N}_{\text{T}} v_{\text{a}}}{4\pi v_{\text{r}} R_{\text{o}}}}{\left(1.5 \times 10^{8} \frac{\text{mol}}{\text{cm}^{3}}\right) \left(1.04 \times 10^{-15} \frac{\text{cm}^{2}}{\text{mol}}\right) \left(1.76 \times 10^{22} \frac{\text{mol}}{\text{sec}}\right) \left(8 \times 10^{5} \frac{\text{cm}}{\text{sec}}\right)}{4\pi (10^{5} \text{ cm/sec}) (1370 \text{ cm})}$$

This is two orders of magnitude less than the impingement of atmospheric molecules.

CONCLUSIONS AND RECOMMENDATIONS

The expulsion of 100 lb/day of fuel cell water through a supersonic nozzle directed along the x-axis will result in column densities greater than 10^{12} molecules/cm² only when viewing at angles less than 48 deg from the tail. Smaller viewing angles could be achieved by canting the nozzle slightly downward. The effect of accumulation of $\rm H_2O$ in the orbital path is negligible. Even if the $\rm H_2O$ plume were directed into the velocity vector, the column density from

the backscatter would still be almost an order of magnitude below the 10^{12} molecule/cm² criteria, which, incidentally, is two orders of magnitude smaller than the column density of the residual atmosphere at 420 km.

If the spacecraft is randomly oriented, the return flux from atmospheric backscatter is $\sim 10^{12}$ molecules/cm² sec at the stagnation point. This is considerably less than the flux of atmospheric molecules. If the molecules hit and stick to a cryogenic surface, a monolayer (10^{15} molecules/cm²) will form in 10^3 sec. After 7 days, 600 monolayers would deposit. This is 18 micrograms/cm², or 1 800 Å. This could be avoided by always orienting the nozzle away from the velocity vector or by shielding the cryogenic surface from the velocity vector.

COLUMN DENSITIES RESULTING FROM SHUTTLE SUBLIMATOR/EVAPORATOR OPERATION

By Robert J. Naumann

The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

CHARLES A. LUNDQUIST

Director, Space Sciences Laboratory